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catena-Poly[diethyl(2-hydroxyethyl)-ammonium [[tetra-μ-acetato-κ^8O:O'-dicuprate(II)](*Cu*—*Cu*)]-μ-acetato-κ^2O:O'] dichloromethane solvate]

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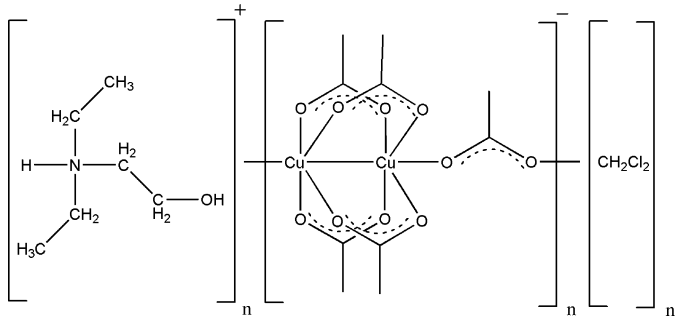
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.034; wR factor = 0.080; data-to-parameter ratio = 19.4.

The title compound, $\{(C_6H_{16}NO)[Cu_2(CH_3COO)_5]\cdot CH_2Cl_2\}_n$, consists of acetate-bridged $Cu_2(CH_3COO)_4$ units that are connected *via* another acetate anion at each terminus to form infinite anionic $[\{Cu_2(CH_3COO)_4\}(CH_3COO)]_n$ chains along [100]. The connecting acetate is hydrogen bonded to the diethyl(2-hydroxyethyl)ammonium cation, and the dichloromethane solvent molecule fills the remaining voids in the structure. The O—Cu—Cu angles along the polymeric chain are nearly linear [175.49 (5)°], but individual O—Cu—Cu—O units along the chain are bent and rotated against each other at the bridging acetate ion. Translation of each $Cu_2(CH_3COO)_4$ unit along the chain, represented by the least-squares plane of the two copper ions along with four of the acetate O atoms, rotated these units by 35.16 (3)°.

Related literature

Shahid, Mazhar, Helliwell *et al.* (2008) describe the study of dinuclear Cu complexes; Van Niekerk & Schoening (1953) provide X-ray evidence for Cu—Cu bonds in cupric acetate; Brown & Chidambaram (1973) report the redetermination of the structure of cupric acetate by neutron-diffraction; Shahid, Mazhar, Malik *et al.* (2008); Hamid *et al.* (2007) and Zhang *et al.* (2004) describe geometric parameters of organo–copper complexes.



Experimental

Crystal data

$(C_6H_{16}NO)[Cu_2(C_2H_3O_2)_5]\cdot CH_2Cl_2$
M_r = 625.42
Orthorhombic, $Pna2_1$
a = 17.6366 (11) Å
b = 12.1078 (8) Å
c = 11.9148 (7) Å
V = 2544.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.94 mm^{-1}
T = 100 (2) K
0.40 × 0.40 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.657, T_{max} = 0.830
21202 measured reflections
5939 independent reflections
5693 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.080
S = 1.08
5939 reflections
306 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Absolute structure: Flack (1983), 2726 Friedel pairs
Flack parameter: 0.017 (11)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O10^{i}	0.93	1.97	2.832 (4)	153
N1—H1···O9^{i}	0.93	2.45	3.056 (3)	123
O11—H11···O9^{i}	0.84	2.04	2.840 (3)	159

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2161).

References

Brown, G. M. & Chidambaram, R. (1973). *Acta Cryst.* B**29**, 2393–2403.
Bruker (2001). *SMART* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Hamid, M., Tahir, A. A., Mazhar, M., Zeller, M. & Hunter, A. D. (2007). *Inorg. Chem.* **46**, 4120–4127.
Shahid, M., Mazhar, M., Helliwell, M., Akhtar, J. & Ahmad, K. (2008). *Acta Cryst.* E**64**, m1139–m1140.
Shahid, M., Mazhar, M., Malik, M. A., O'Brien, P. & Raftery, J. (2008). *Polyhedron*, **27**, 3337–3342.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Van Niekerk, J. N. & Schoening, F. R. L. (1953). *Nature (London)*, **171**, 36–37.
Zhang, Y.-L., Chen, S.-W., Liu, W.-S. & Wang, D.-Q. (2004). *Acta Cryst.* E**60**, m196–m197.

supplementary materials

Acta Cryst. (2009). E**65**, m163-m164 [**doi:10.1107/S1600536808044048**]

catena-Poly[diethyl(2-hydroxyethyl)ammonium [[tetra-μ-acetato-κ^8O:O'-dicuprate(II)(*Cu*-*Cu*)]-μ-acetato-κ^2O:O'] dichloromethane solvate]

M. Shahid, M. Mazhar, P. O'Brien, M. Afzaal and J. Raftery

Comment

The background of this study has been set out in our previous work on the structural chemistry of metal-organic compounds (Shahid, Mazhar, Helliwell *et al.*, 2008). Herein, as a continuation of these studies, the structure of the title compound is described which consists of acetate bridged $Cu_2(CH_3COO)_4$ units that are connected *via* another acetate anion at each terminus to form infinite anionic $[\{Cu_2(CH_3COO)_4\}(CH_3COO)]_n$ chains along the [100] direction of the crystal. Crystallographically speaking the chain is generated from *a* glide related copies of the monomer. The connecting acetate is hydrogen bonded to the (diethylammonium)ethanol cation (Fig. 2). The dichloromethane solvate molecule occupies voids in the structure. The O—Cu—Cu angles along the polymeric chain are nearly linear (175.49 (5)°), but individual O—Cu—Cu—O units along the chain are rotated relative to each other. Representing the orientation of $Cu_2(CH_3COO)_4$ unit by the least squares plane Cu1 Cu2 O1 O2 O5 O6, translation along the chain rotates the orientation by 35.16 (3)°.

In the title compound (Fig.1), the two metal centers are similar; each has a coordination number of six having a coordination geometry close to octahedral, with a CuO_5Cu core similar to that of Cu centers in $Cu_2(OAc)_4(H_2O)_2$. The basal planes of Cu(1) and Cu(2) are each composed of an oxygen from each of the four acetate groups (O(1), O(3), O(5), O(8) and O(2), O(4), O(6), O(7) respectively), which link the two copper atoms in the monomer. Coordination by the fifth acetate's O atoms, O(9) and O(10) (from a symmetry generated copy), form one apical bond for Cu(2) and Cu(1) respectively. The octahedral coordination of the copper atoms is completed by the apical Cu(1)—Cu(2) bond of 2.6259 (4) Å. This is significantly shorter than the 2.64 Å as reported for dinuclear copper (II) acetate monohydrate in 1953 (Van Niekerk & Schoening, 1953), but close to the more accurate value obtained in a redetermination by neutron diffraction analysis (2.6143 (17) Å, Brown & Chidambaram, 1973). The Cu—O bond lengths in the basal planes for both the Cu atoms range from 1.949 (2) to 1.985 (2) Å and the average distance is in good agreement with 1.97 Å, as reported for copper acetate (Van Niekerk & Schoening, 1953). The most striking structural difference between the title compound and the dinuclear units in cupric acetate appears to be the weaker apixal bonds Cu—O which are 2.148 (18) and 2.124 (18) Å for Cu(1) and Cu(2), respectively in the title compound and 2.20 Å in the cupric acetate. The distortion is further evident from the slight deviation of *trans* angles in the basal plane and axial angle from ideal value of 180°. This is in good agreement with the literature (Shahid, Mazhar, Malik *et al.*, 2008); Hamid *et al.*, 2007; Zhang *et al.*, 2004). In the structure, the (diethylamonium)ethanol cations are linked through hydrogen bonds [O(11)—H(11)···O(9)], [N(1)—H(1)···O(9)] and [N(1)—H(1)···O(10)] to the connecting acetate group occupying *cis* positions at the main polymeric chain (Table 1, Fig. 3).

Experimental

N,*N*-Diethylaminoethanol (deaeH) (0.27 g, 2.34 mmol) and acetic acid (0.14 g, 2.34 mmol) were added to a stirred suspension of $Cu(CH_3COO)_2.H_2O$ (0.85 g, 4.67 mmol) in 25 ml dichloromethane. After two hours stirring, the mixture was vacu-

um evaporated to dryness and the solid was redissolved in minimum amount of dichloromethane to give blue block-shaped crystals at room temperature after two weeks.

Refinement

The non-hydrogen atoms were refined anisotropically. H atoms were included in calculated positions with C—H lengths of 0.95(CH), 0.99(CH_2) & 0.98(CH_3)Å; U_{iso}(H) values were fixed at 1.2U_{eq}(C) except for CH_3 where it was 1.5U_{eq}(C). For N—H and O—H the lengths and U_{iso} were 0.98Å and 1.2U_{eq}(N) and 0.84Å and 1.5U_{eq}(O) respectively.

Figures

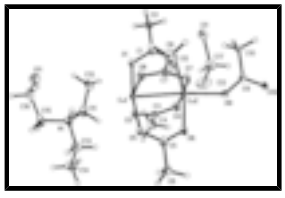

Fig. 1. View of the title compound (50% probability displacement ellipsoids)

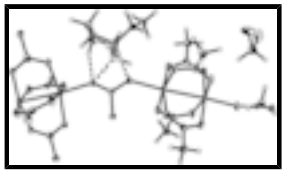

Fig. 2. Fragment of the chain showing the H-bonding interactions.

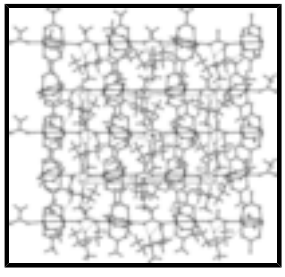

Fig. 3. View down the **b** axis showing the infinite chains.

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Crystal data

$(C_6H_{16}NO)[Cu_2(C_2H_3O_2)_5]\cdot CH_2Cl_2$	D_x = 1.633 Mg m^{-3}
M_r = 625.42	Mo *K*α radiation λ = 0.71073 Å
Orthorhombic, *Pna*2$_1$	Cell parameters from 7814 reflections
a = 17.6366 (11) Å	θ = 2.4–28.1°
b = 12.1078 (8) Å	μ = 1.94 mm^{-1}
c = 11.9148 (7) Å	*T* = 100 (2) K
V = 2544.3 (3) Å^3	Plate, turquoise
Z = 4	0.40 × 0.40 × 0.10 mm
F_{000} = 1288	

Data collection

Bruker SMART CCD area-detector diffractometer	5939 independent reflections
Radiation source: fine-focus sealed tube	5693 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.029$
$T = 100(2)$ K	$\theta_{max} = 28.3°$
φ and ω scans	$\theta_{min} = 2.0°$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -22 \rightarrow 22$
$T_{min} = 0.657$, $T_{max} = 0.830$	$k = -16 \rightarrow 15$
21202 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.034$	$w = 1/[\sigma^2(F_o^2) + (0.0393P)^2 + 1.2652P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.080$	$(\Delta/\sigma)_{max} = 0.013$
$S = 1.08$	$\Delta\rho_{max} = 0.75$ e Å^{-3}
5939 reflections	$\Delta\rho_{min} = -0.40$ e Å^{-3}
306 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 2726 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.017 (11)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O10	1.03029 (10)	0.66475 (16)	0.5408 (2)	0.0152 (4)
C1	0.75148 (17)	0.9544 (3)	0.6165 (2)	0.0176 (6)
C2	0.77083 (18)	1.0672 (3)	0.6609 (3)	0.0206 (6)

H2A	0.7588	1.0707	0.7411	0.031*
H2B	0.7413	1.1230	0.6206	0.031*
H2C	0.8250	1.0813	0.6500	0.031*
C3	0.73249 (17)	0.8234 (2)	0.3482 (2)	0.0166 (6)
C4	0.73934 (19)	0.8662 (3)	0.2292 (3)	0.0222 (7)
H4A	0.7896	0.8478	0.1994	0.033*
H4B	0.7327	0.9465	0.2289	0.033*
H4C	0.7002	0.8319	0.1823	0.033*
C5	0.68347 (17)	0.5689 (3)	0.4849 (3)	0.0191 (6)
C6	0.66262 (19)	0.4540 (3)	0.4463 (3)	0.0283 (8)
H6A	0.7085	0.4087	0.4414	0.042*
H6B	0.6384	0.4581	0.3724	0.042*
H6C	0.6274	0.4208	0.5002	0.042*
C7	0.71363 (17)	0.6985 (3)	0.7522 (3)	0.0173 (6)
C8	0.71030 (19)	0.6623 (3)	0.8732 (3)	0.0257 (7)
H8A	0.6693	0.7017	0.9116	0.039*
H8B	0.7587	0.6791	0.9100	0.039*
H8C	0.7008	0.5826	0.8767	0.039*
C9	0.96959 (15)	0.7062 (2)	0.5798 (2)	0.0133 (6)
C10	0.97463 (17)	0.7894 (3)	0.6744 (3)	0.0189 (6)
H10A	1.0156	0.7682	0.7256	0.028*
H10B	0.9265	0.7909	0.7154	0.028*
H10C	0.9851	0.8628	0.6433	0.028*
C11	0.54065 (17)	0.9990 (3)	0.2860 (3)	0.0210 (7)
H11A	0.5795	0.9515	0.2504	0.025*
H11B	0.5183	1.0463	0.2268	0.025*
C12	0.57806 (18)	1.0711 (3)	0.3723 (3)	0.0240 (7)
H12A	0.5967	1.0253	0.4342	0.036*
H12B	0.5412	1.1246	0.4012	0.036*
H12C	0.6206	1.1106	0.3379	0.036*
C13	0.4783 (2)	0.8130 (3)	0.2850 (3)	0.0265 (7)
H13A	0.4413	0.7669	0.3262	0.032*
H13B	0.5290	0.7792	0.2947	0.032*
C14	0.4581 (2)	0.8124 (4)	0.1617 (3)	0.0350 (9)
H14A	0.4934	0.8599	0.1205	0.052*
H14B	0.4063	0.8399	0.1519	0.052*
H14C	0.4615	0.7368	0.1327	0.052*
C15	0.40137 (17)	0.9772 (3)	0.3296 (3)	0.0249 (7)
H15A	0.3913	0.9998	0.2512	0.030*
H15B	0.3635	0.9203	0.3499	0.030*
C16	0.39024 (18)	1.0753 (3)	0.4043 (3)	0.0280 (7)
H16A	0.4225	1.1365	0.3771	0.034*
H16B	0.3368	1.0996	0.3991	0.034*
C17	0.9547 (2)	0.9492 (3)	0.4356 (3)	0.0292 (8)
H17A	0.9991	0.9018	0.4520	0.035*
H17B	0.9086	0.9093	0.4601	0.035*
Cl1	0.96272 (5)	1.07456 (9)	0.51185 (9)	0.0367 (2)
Cl2	0.94975 (7)	0.97421 (9)	0.29049 (9)	0.0475 (3)
Cu1	0.647405 (16)	0.78765 (2)	0.55145 (3)	0.01289 (8)

Cu2	0.791704 (16)	0.73425 (3)	0.54933 (4)	0.01346 (8)
N1	0.47907 (14)	0.9266 (2)	0.3355 (2)	0.0182 (5)
H1	0.4905	0.9179	0.4112	0.022*
O1	0.68332 (11)	0.93608 (17)	0.59168 (18)	0.0168 (4)
O2	0.80508 (12)	0.88517 (18)	0.60953 (19)	0.0211 (5)
O3	0.66724 (12)	0.82111 (19)	0.39116 (18)	0.0184 (4)
O4	0.79321 (12)	0.79520 (19)	0.39662 (19)	0.0194 (5)
O5	0.62993 (11)	0.63224 (17)	0.51139 (19)	0.0193 (4)
O6	0.75254 (11)	0.59322 (18)	0.4873 (2)	0.0202 (5)
O7	0.77446 (12)	0.67809 (19)	0.70047 (19)	0.0212 (5)
O8	0.65654 (12)	0.7454 (2)	0.71140 (18)	0.0188 (4)
O9	0.90593 (10)	0.67911 (16)	0.5416 (2)	0.0172 (4)
O11	0.40773 (14)	1.05419 (19)	0.5170 (2)	0.0306 (6)
H11	0.3963	0.9886	0.5327	0.046*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O10	0.0095 (8)	0.0212 (9)	0.0148 (10)	−0.0006 (6)	0.0011 (8)	−0.0015 (10)
C1	0.0178 (15)	0.0243 (16)	0.0107 (14)	−0.0011 (12)	0.0035 (11)	0.0009 (12)
C2	0.0197 (15)	0.0206 (16)	0.0215 (15)	−0.0048 (12)	0.0025 (13)	−0.0057 (12)
C3	0.0190 (14)	0.0160 (14)	0.0148 (14)	−0.0009 (11)	−0.0020 (12)	−0.0026 (11)
C4	0.0220 (16)	0.0293 (17)	0.0153 (15)	0.0007 (13)	0.0025 (12)	0.0042 (13)
C5	0.0186 (15)	0.0205 (15)	0.0182 (15)	0.0010 (12)	0.0025 (12)	0.0014 (12)
C6	0.0172 (16)	0.0200 (16)	0.048 (2)	−0.0038 (12)	0.0046 (15)	−0.0101 (15)
C7	0.0172 (15)	0.0179 (14)	0.0168 (15)	−0.0019 (11)	0.0000 (11)	−0.0016 (12)
C8	0.0232 (16)	0.0366 (19)	0.0173 (16)	0.0060 (14)	0.0024 (13)	0.0091 (14)
C9	0.0139 (13)	0.0139 (13)	0.0123 (15)	−0.0011 (10)	−0.0003 (10)	0.0017 (9)
C10	0.0144 (14)	0.0209 (16)	0.0213 (16)	0.0000 (11)	−0.0036 (12)	−0.0091 (12)
C11	0.0150 (15)	0.0296 (18)	0.0185 (16)	−0.0010 (12)	0.0033 (12)	0.0075 (13)
C12	0.0144 (15)	0.0294 (17)	0.0283 (17)	−0.0048 (13)	−0.0006 (13)	0.0063 (14)
C13	0.0315 (19)	0.0241 (16)	0.0240 (17)	−0.0013 (14)	−0.0016 (14)	0.0000 (14)
C14	0.040 (2)	0.043 (2)	0.0215 (17)	−0.0088 (17)	−0.0011 (16)	−0.0045 (16)
C15	0.0135 (15)	0.0404 (19)	0.0208 (16)	−0.0001 (13)	−0.0038 (12)	0.0141 (14)
C16	0.0133 (15)	0.0298 (17)	0.041 (2)	0.0028 (13)	0.0025 (14)	0.0116 (15)
C17	0.0277 (18)	0.036 (2)	0.0242 (18)	−0.0045 (14)	0.0010 (15)	0.0061 (15)
Cl1	0.0248 (4)	0.0460 (5)	0.0393 (5)	0.0034 (4)	−0.0039 (4)	−0.0083 (4)
Cl2	0.0826 (8)	0.0327 (5)	0.0272 (5)	−0.0082 (5)	0.0083 (5)	0.0062 (4)
Cu1	0.00720 (13)	0.01831 (15)	0.01316 (15)	0.00109 (10)	0.00003 (17)	−0.00089 (17)
Cu2	0.00722 (13)	0.01905 (15)	0.01411 (15)	0.00129 (10)	0.00009 (19)	−0.00129 (18)
N1	0.0148 (12)	0.0255 (14)	0.0142 (12)	−0.0033 (10)	−0.0022 (10)	0.0056 (11)
O1	0.0117 (10)	0.0184 (10)	0.0205 (10)	0.0008 (8)	−0.0007 (8)	−0.0027 (8)
O2	0.0119 (10)	0.0253 (12)	0.0260 (12)	0.0025 (9)	−0.0020 (9)	−0.0077 (10)
O3	0.0117 (10)	0.0290 (12)	0.0145 (10)	0.0008 (9)	−0.0004 (8)	0.0014 (9)
O4	0.0127 (10)	0.0295 (12)	0.0161 (11)	0.0003 (8)	0.0025 (8)	0.0018 (9)
O5	0.0123 (10)	0.0200 (10)	0.0255 (11)	−0.0005 (8)	−0.0006 (8)	−0.0045 (8)
O6	0.0103 (10)	0.0207 (11)	0.0295 (13)	−0.0016 (8)	0.0002 (9)	−0.0022 (9)
O7	0.0138 (10)	0.0317 (12)	0.0183 (11)	0.0069 (9)	0.0001 (9)	0.0054 (9)

O8	0.0153 (10)	0.0273 (12)	0.0137 (10)	0.0043 (9)	0.0023 (8)	0.0023 (9)
O9	0.0083 (8)	0.0220 (9)	0.0213 (11)	0.0002 (7)	−0.0008 (10)	−0.0075 (10)
O11	0.0310 (13)	0.0231 (11)	0.0378 (15)	−0.0031 (10)	0.0034 (11)	−0.0001 (10)

Geometric parameters (Å, °)

O10—C9	1.271 (3)	C12—H12A	0.9800
O10—Cu1^{i}	2.1482 (18)	C12—H12B	0.9800
C1—O1	1.258 (4)	C12—H12C	0.9800
C1—O2	1.266 (4)	C13—N1	1.500 (4)
C1—C2	1.504 (4)	C13—C14	1.512 (5)
C2—H2A	0.9800	C13—H13A	0.9900
C2—H2B	0.9800	C13—H13B	0.9900
C2—H2C	0.9800	C14—H14A	0.9800
C3—O3	1.260 (4)	C14—H14B	0.9800
C3—O4	1.263 (4)	C14—H14C	0.9800
C3—C4	1.514 (4)	C15—C16	1.496 (5)
C4—H4A	0.9800	C15—N1	1.503 (4)
C4—H4B	0.9800	C15—H15A	0.9900
C4—H4C	0.9800	C15—H15B	0.9900
C5—O6	1.254 (4)	C16—O11	1.400 (4)
C5—O5	1.257 (4)	C16—H16A	0.9900
C5—C6	1.510 (4)	C16—H16B	0.9900
C6—H6A	0.9800	C17—Cl2	1.758 (4)
C6—H6B	0.9800	C17—Cl1	1.775 (4)
C6—H6C	0.9800	C17—H17A	0.9900
C7—O8	1.254 (4)	C17—H17B	0.9900
C7—O7	1.262 (4)	Cu1—O1	1.965 (2)
C7—C8	1.508 (4)	Cu1—O5	1.966 (2)
C8—H8A	0.9800	Cu1—O8	1.980 (2)
C8—H8B	0.9800	Cu1—O3	1.983 (2)
C8—H8C	0.9800	Cu1—O10^{ii}	2.1482 (18)
C9—O9	1.255 (3)	Cu1—Cu2	2.6259 (4)
C9—C10	1.514 (4)	Cu2—O7	1.949 (2)
C10—H10A	0.9800	Cu2—O4	1.964 (2)
C10—H10B	0.9800	Cu2—O2	1.977 (2)
C10—H10C	0.9800	Cu2—O6	1.985 (2)
C11—C12	1.502 (5)	Cu2—O9	2.1243 (18)
C11—N1	1.515 (4)	N1—H1	0.9300
C11—H11A	0.9900	O11—H11	0.8400
C11—H11B	0.9900		
C9—O10—Cu1^{i}	133.03 (19)	C13—C14—H14C	109.5
O1—C1—O2	125.5 (3)	H14A—C14—H14C	109.5
O1—C1—C2	117.4 (3)	H14B—C14—H14C	109.5
O2—C1—C2	117.1 (3)	C16—C15—N1	114.6 (3)
C1—C2—H2A	109.5	C16—C15—H15A	108.6
C1—C2—H2B	109.5	N1—C15—H15A	108.6
H2A—C2—H2B	109.5	C16—C15—H15B	108.6

C1—C2—H2C	109.5	N1—C15—H15B	108.6
H2A—C2—H2C	109.5	H15A—C15—H15B	107.6
H2B—C2—H2C	109.5	O11—C16—C15	113.4 (3)
O3—C3—O4	125.6 (3)	O11—C16—H16A	108.9
O3—C3—C4	117.4 (3)	C15—C16—H16A	108.9
O4—C3—C4	116.9 (3)	O11—C16—H16B	108.9
C3—C4—H4A	109.5	C15—C16—H16B	108.9
C3—C4—H4B	109.5	H16A—C16—H16B	107.7
H4A—C4—H4B	109.5	Cl2—C17—Cl1	111.1 (2)
C3—C4—H4C	109.5	Cl2—C17—H17A	109.4
H4A—C4—H4C	109.5	Cl1—C17—H17A	109.4
H4B—C4—H4C	109.5	Cl2—C17—H17B	109.4
O6—C5—O5	125.5 (3)	Cl1—C17—H17B	109.4
O6—C5—C6	117.4 (3)	H17A—C17—H17B	108.0
O5—C5—C6	117.1 (3)	O1—Cu1—O5	170.19 (8)
C5—C6—H6A	109.5	O1—Cu1—O8	88.59 (10)
C5—C6—H6B	109.5	O5—Cu1—O8	89.95 (10)
H6A—C6—H6B	109.5	O1—Cu1—O3	89.50 (9)
C5—C6—H6C	109.5	O5—Cu1—O3	89.39 (10)
H6A—C6—H6C	109.5	O8—Cu1—O3	164.87 (9)
H6B—C6—H6C	109.5	O1—Cu1—O10^{ii}	94.53 (8)
O8—C7—O7	125.6 (3)	O5—Cu1—O10^{ii}	95.26 (8)
O8—C7—C8	118.1 (3)	O8—Cu1—O10^{ii}	101.81 (9)
O7—C7—C8	116.3 (3)	O3—Cu1—O10^{ii}	93.31 (9)
C7—C8—H8A	109.5	O1—Cu1—Cu2	85.13 (6)
C7—C8—H8B	109.5	O5—Cu1—Cu2	85.06 (6)
H8A—C8—H8B	109.5	O8—Cu1—Cu2	82.34 (6)
C7—C8—H8C	109.5	O3—Cu1—Cu2	82.54 (6)
H8A—C8—H8C	109.5	O10^{ii}—Cu1—Cu2	175.83 (7)
H8B—C8—H8C	109.5	O7—Cu2—O4	171.68 (9)
O9—C9—O10	121.2 (3)	O7—Cu2—O2	90.33 (10)
O9—C9—C10	119.7 (2)	O4—Cu2—O2	89.27 (10)
O10—C9—C10	119.1 (2)	O7—Cu2—O6	89.42 (10)
C9—C10—H10A	109.5	O4—Cu2—O6	89.01 (10)
C9—C10—H10B	109.5	O2—Cu2—O6	166.35 (9)
H10A—C10—H10B	109.5	O7—Cu2—O9	94.49 (9)
C9—C10—H10C	109.5	O4—Cu2—O9	93.75 (9)
H10A—C10—H10C	109.5	O2—Cu2—O9	101.13 (8)
H10B—C10—H10C	109.5	O6—Cu2—O9	92.50 (8)
C12—C11—N1	112.6 (3)	O7—Cu2—Cu1	85.74 (6)
C12—C11—H11A	109.1	O4—Cu2—Cu1	85.95 (6)
N1—C11—H11A	109.1	O2—Cu2—Cu1	83.37 (6)
C12—C11—H11B	109.1	O6—Cu2—Cu1	83.00 (6)
N1—C11—H11B	109.1	O9—Cu2—Cu1	175.49 (5)
H11A—C11—H11B	107.8	C13—N1—C15	110.3 (3)
C11—C12—H12A	109.5	C13—N1—C11	112.4 (3)
C11—C12—H12B	109.5	C15—N1—C11	113.5 (3)
H12A—C12—H12B	109.5	C13—N1—H1	106.7

C11—C12—H12C	109.5	C15—N1—H1	106.7
H12A—C12—H12C	109.5	C11—N1—H1	106.7
H12B—C12—H12C	109.5	C1—O1—Cu1	121.79 (19)
N1—C13—C14	113.4 (3)	C1—O2—Cu2	123.1 (2)
N1—C13—H13A	108.9	C3—O3—Cu1	123.84 (19)
C14—C13—H13A	108.9	C3—O4—Cu2	120.88 (19)
N1—C13—H13B	108.9	C5—O5—Cu1	121.84 (19)
C14—C13—H13B	108.9	C5—O6—Cu2	123.3 (2)
H13A—C13—H13B	107.7	C7—O7—Cu2	121.1 (2)
C13—C14—H14A	109.5	C7—O8—Cu1	123.7 (2)
C13—C14—H14B	109.5	C9—O9—Cu2	138.64 (19)
H14A—C14—H14B	109.5	C16—O11—H11	109.5
Cu1^{i}—O10—C9—O9	163.2 (2)	O8—Cu1—O3—C3	−7.4 (5)
Cu1^{i}—O10—C9—C10	−17.2 (4)	O10^{ii}—Cu1—O3—C3	169.8 (2)
N1—C15—C16—O11	−54.5 (4)	Cu2—Cu1—O3—C3	−9.9 (2)
O1—Cu1—Cu2—O7	97.97 (10)	O3—C3—O4—Cu2	3.4 (4)
O5—Cu1—Cu2—O7	−81.87 (10)	C4—C3—O4—Cu2	−178.2 (2)
O8—Cu1—Cu2—O7	8.74 (10)	O2—Cu2—O4—C3	−91.6 (2)
O3—Cu1—Cu2—O7	−171.90 (10)	O6—Cu2—O4—C3	74.9 (2)
O1—Cu1—Cu2—O4	−82.60 (9)	O9—Cu2—O4—C3	167.3 (2)
O5—Cu1—Cu2—O4	97.56 (10)	Cu1—Cu2—O4—C3	−8.2 (2)
O8—Cu1—Cu2—O4	−171.83 (10)	O6—C5—O5—Cu1	4.7 (4)
O3—Cu1—Cu2—O4	7.53 (9)	C6—C5—O5—Cu1	−175.0 (2)
O1—Cu1—Cu2—O2	7.13 (9)	O8—Cu1—O5—C5	−91.6 (2)
O5—Cu1—Cu2—O2	−172.71 (10)	O3—Cu1—O5—C5	73.3 (2)
O8—Cu1—Cu2—O2	−82.10 (10)	O10^{ii}—Cu1—O5—C5	166.5 (2)
O3—Cu1—Cu2—O2	97.26 (10)	Cu2—Cu1—O5—C5	−9.3 (2)
O1—Cu1—Cu2—O6	−172.10 (10)	O5—C5—O6—Cu2	6.5 (4)
O5—Cu1—Cu2—O6	8.06 (9)	C6—C5—O6—Cu2	−173.8 (2)
O8—Cu1—Cu2—O6	98.67 (10)	O7—Cu2—O6—C5	75.7 (2)
O3—Cu1—Cu2—O6	−81.97 (10)	O4—Cu2—O6—C5	−96.2 (2)
C14—C13—N1—C15	62.7 (4)	O2—Cu2—O6—C5	−13.3 (6)
C14—C13—N1—C11	−65.1 (4)	O9—Cu2—O6—C5	170.1 (2)
C16—C15—N1—C13	163.9 (3)	Cu1—Cu2—O6—C5	−10.1 (2)
C16—C15—N1—C11	−68.9 (3)	O8—C7—O7—Cu2	7.2 (4)
C12—C11—N1—C13	−141.1 (3)	C8—C7—O7—Cu2	−173.0 (2)
C12—C11—N1—C15	92.8 (3)	O2—Cu2—O7—C7	72.4 (2)
O2—C1—O1—Cu1	6.5 (4)	O6—Cu2—O7—C7	−94.0 (2)
C2—C1—O1—Cu1	−171.9 (2)	O9—Cu2—O7—C7	173.6 (2)
O8—Cu1—O1—C1	73.2 (2)	Cu1—Cu2—O7—C7	−11.0 (2)
O3—Cu1—O1—C1	−91.8 (2)	O7—C7—O8—Cu1	4.9 (5)
O10^{ii}—Cu1—O1—C1	174.9 (2)	C8—C7—O8—Cu1	−174.9 (2)
Cu2—Cu1—O1—C1	−9.2 (2)	O1—Cu1—O8—C7	−95.1 (3)
O1—C1—O2—Cu2	3.4 (4)	O5—Cu1—O8—C7	75.2 (3)
C2—C1—O2—Cu2	−178.2 (2)	O3—Cu1—O8—C7	−12.3 (6)
O7—Cu2—O2—C1	−93.5 (2)	O10^{ii}—Cu1—O8—C7	170.5 (2)
O4—Cu2—O2—C1	78.2 (2)	Cu2—Cu1—O8—C7	−9.9 (2)
O6—Cu2—O2—C1	−4.6 (6)	O10—C9—O9—Cu2	−166.8 (2)

O9—Cu2—O2—C1	171.9 (2)	C10—C9—O9—Cu2	13.5 (5)
Cu1—Cu2—O2—C1	−7.8 (2)	O7—Cu2—O9—C9	−75.7 (3)
O4—C3—O3—Cu1	7.0 (4)	O4—Cu2—O9—C9	105.5 (3)
C4—C3—O3—Cu1	−171.4 (2)	O2—Cu2—O9—C9	15.5 (3)
O1—Cu1—O3—C3	75.3 (2)	O6—Cu2—O9—C9	−165.4 (3)
O5—Cu1—O3—C3	−94.9 (2)		

Symmetry codes: (i) *x*+1/2, −*y*+3/2, *z*; (ii) *x*−1/2, −*y*+3/2, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O10^{ii}	0.93	1.97	2.832 (4)	153
N1—H1···O9^{ii}	0.93	2.45	3.056 (3)	123
O11—H11···O9^{ii}	0.84	2.04	2.840 (3)	159

Symmetry codes: (ii) *x*−1/2, −*y*+3/2, *z*.

Fig. 1

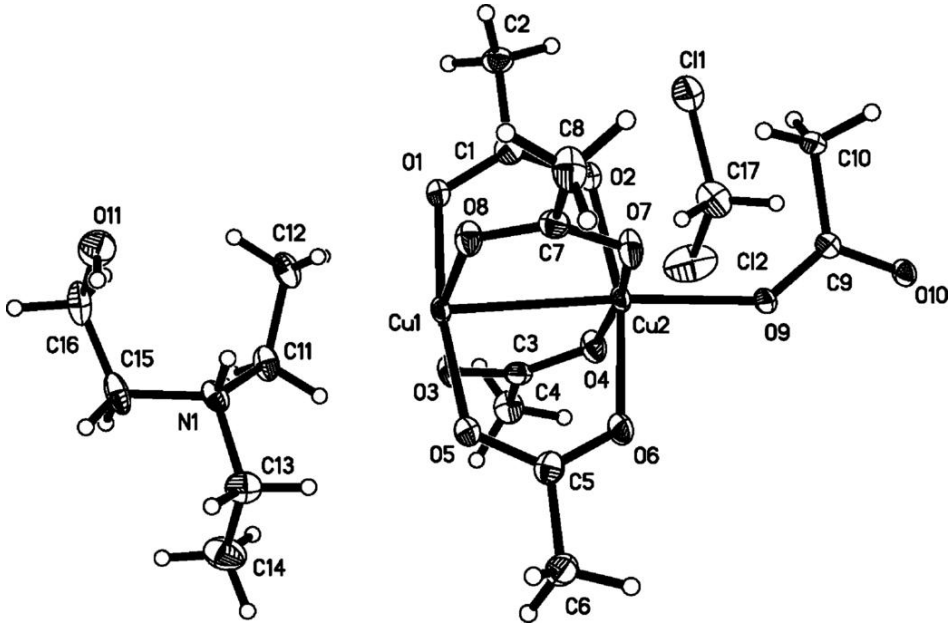
C2
Cl1
C8
C1
O1
O2
C17
C10
O8
O7
C7
Cl2
C9
O10
O11
C12
Cu1
Cu2
O9
C16
C15
C11
C3
O4
O3
C4
N1
O5
O6
C13
C5
C14
C6

Fig. 2

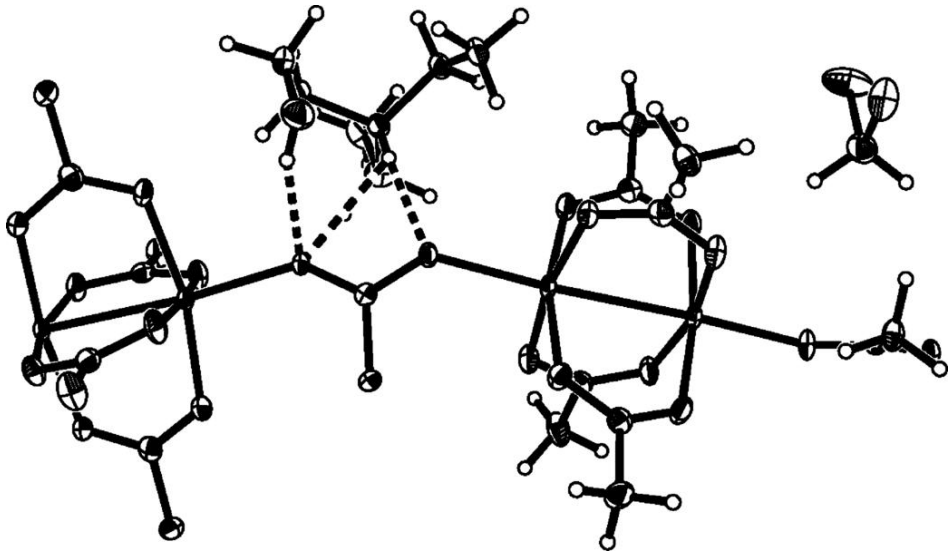

Fig. 3